On the Crucial Significance of the Multi-Configuration Structure of a Bound State of Several Dirac Particles

E. Comay*

Charactell Ltd.

P.O. Box 39019, Tel Aviv 61390

Israel

PACS No: 03.65.Ge

Abstract:

The structure of a bound state of several Dirac particles is discussed. Relying on solid mathematical arguments of the Wigner-Racah algebra, it is proved the a non-negligible number of configurations is required for a description of this kind of systems. At present, the main results are not widely known and this is the underlying reason for the phenomenon called the proton spin crisis.

1. Introduction

Once upon a midnight dreary, while I pondered weak and weary,

Over many a quaint and curious volume of forgotten lore...[1].

The objective if this work is to prove that the multi-configuration structure of a bound state of several Dirac particles plays an extremely important role. The existence of such a multi-configuration structure was already known many decades ago [2,3] and early electronic computers were used for providing a numerical proof of this issue [4]. (Note that the first edition of [2] was published in 1935.) Unfortunately, this scientific evidence has not found its way to contemporary textbooks of physics [5] and has become a kind of a forgotten lore. The paper proves the main points of this issue and shows its far reaching meaning and its relevance to physical problems that are still unsettled. In doing so the paper aims to make a contribution to the correction of this situation.

It is well known that quantum mechanics explains the Mendeleev periodic table of chemical elements. The shell structure of electrons provides an easy interpretation of chemical properties of noble gases (a full shell), halogens (a full shell minus 1), alkali metals (a full shell + 1) etc. The standard explanation of the Mendeleev periodic table uses a single configuration for a description of the electronic states of each chemical element. Thus, for example, the helium and the lithium atoms are described by the $1s^2$ and $1s^22s$ configurations, respectively. At this point the following problem arises: Does the unique configuration structure of an atomic ground state make an acceptable description of its quantum mechanical system or is it just a useful pedagogical explanation of the Mendeleev periodic table? The answer to this problem certainly must be obtained from a mathematical analysis of the quantum mechanical state of systems that contain more than one electron. By describing an outline of

this task, the present work proves beyond any doubt that an atomic state of more than one electron has a multi-configuration structure and that no single configuration dominates the system.

The conclusion stated above has two important aspects. First, It is clear that a correct understanding of the structure of any fundamental physical system is a vital theoretical asset for every physicist. Next, it turns out that the lack of an adequate awareness of this physical evidence has already caused the phenomenon called the "proton spin crisis" [6] which haunts the community for decades. The measurements published in [6] show that quarks carry a very small portion of the proton's spin and this evidence has been regarded as a surprise. Now, it is shown in this work that the multiconfiguration structure found in atomic states is not a specific property of the Coulomb interaction. Thus, it is expected to be also found in any bound state of three spin 1/2 quarks, like it is found in bound states of several spin 1/2 electrons. For this reason, one can state that if the experiment described in [6] would have shown that *quarks carry the entire proton's spin then this result should have been regarded as a real crisis of fundamental quantum mechanical principles.*

In this work, units where $\hbar = c = 1$ are used. The second section contains a brief description of the main properties of a bound state of several Dirac particles that are required for the discussion. The underlying mathematical reasons for the multiconfiguration structure of states are discussed in the third section. Some aspects of the results are pointed out in the last section.

2. General Arguments

The main objective of this work is to find a reliable mathematical method for describing the ground state of a bound system of spin 1/2 particles. Applying Wigner's

analysis of the Poincare group [7,8], one concludes that the total mass (namely, energy) and the total spin are good quantum numbers. Thus, one assumes that an energy operator (namely, a Hamiltonian) exists. For this reason, one can construct a Hilbert space of functions that can be used for describing the given system as an eigenfunction of the Hamiltonian. Evidently, in the system's rest frame, an energy eigenfunction has the time dependent factor $\exp(-iEt)$. This factor can be removed and the basis of the Hilbert space contains time independent functions.

The fact that every relatively stable state has a well defined total spin J can be used for making a considerable simplification of the problem. Thus, one uses a basis for the Hilbert space that is made of functions that have the required spin J and ignores all functions that do not satisfy this condition. Evidently, a smaller Hilbert space reduces the amount of technical work needed for finding the Hamiltonian's eigenfunctions. An additional argument holds for systems whose state is determined by a parity conserving interaction, like the strong and the electromagnetic interactions. Thus, one can use functions that have a well defined parity and build the Hilbert space only from functions that have the required parity. This procedure makes a further simplification of the problem.

The notion of a configuration of a system of several Dirac particles is a useful mathematical tool that satisfies the two requirements stated above (see [2], p. 113 and [9], p. 245). A configuration is written in the form of a product of single particle wave functions describing the corresponding radial and orbital state of each particle belonging to the system (the m quantum number is ignored). For atomic systems a non-relativistic notation is commonly used and the values of the nl quantum numbers denote a configuration, like $1s^2 2s^1$. In relativistic cases the variables nlj (see [9], p. 245) are used. In the latter case, the variables nj^π (here π denotes parity and it takes the values ± 1) is an equivalent notation for a relativistic configuration because $l = j \pm 1/2$ and the numerical parity of the l-value of a Dirac spinor upper part

defines the single particle's parity. (This work uses the nj^{π} notation.) Evidently, any acceptable configuration must be consistent with the Pauli exclusion principle.

For any given state where the total spin J and parity are given, one can use configurations that are consistent with J and the product of the single-particle parity equals the parity of the system. The total angular momentum J is obtained from an application of the law of vector addition of angular momentum (see [2], p. 56 and [9], p. 95). Here the triangular condition holds (see [9], p. 98). Thus, for example, an acceptable configuration for the two-electron 0^+ ground state of the helium atom must take the form $n_1 j_1^{\pi_1}\, n_2 j_2^{\pi_2}$, where $j_1 = j_2$ and $\pi_1 = \pi_2$. Similarly, a description of a 2-electron state where $J^{\pi} = 3^+$ *cannot* contain a configuration of the form $n_1 \frac{1}{2}^+\, n_2 \frac{3}{2}^+$, because the two J values $1/2$ and $3/2$ can only yield a total $J = 1$ or $J = 2$.

At this point the structure of the relevant Hilbert space is known. It is made of configurations that satisfy certain requirements. This is one of the useful properties of using configurations - the relevant Hilbert space is smaller because many configurations can be ignored due to the total spin and parity requirements. Obviously, a smaller Hilbert space means shorter computational efforts. Thus, the framework needed for the analysis is established. The problem of finding how many configurations are required for an acceptable description of an atomic state is discussed in the following section.

3. The Multi-Configuration Structure of Atomic States

The purpose of this section is to outline a proof that shows why a bound state of several electrons takes the form of a linear combination of configurations. For this purpose, the Hamiltonian matrix is constructed for a Hilbert space whose basis is made of functions that take a configuration form. Evidently, non-vanishing off-

diagonal matrix elements prove that the required state is a linear combination of configurations. It is shown that this property holds even for the simplest atomic state of more than one electron, namely the $J^\pi = 0^+$ ground state of the 2-electron Helium atom.

As stated in the previous section, the required Hilbert space contains functions that have the given total spin and parity. The form of a two electron function is written as follows

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = F_i(r_1)F_k(r_2)(j_1^{\pi_1} j_2^{\pi_2} JM). \tag{1}$$

Here, $F_i(r_1)$, $F_k(r_2)$ denote radial functions of the corresponding electron, j_1, j_2, π_1, π_2 denote the single particle spin and parity of the electrons, respectively, J is the total spin obtained by using the appropriate Clebsch-Gordan coefficients [2,9] and M denotes the magnetic quantum number of the total angular momentum,

Let us use the principles described in the previous section and try to find the structure of the helium atom ground state. Thus, due to the triangular rule (see [9], p. 98) and in order to be consistent with $J = 0$, we must use configurations where $j_1 = j_2$. Similarly, in order to have an even total parity, we must use configurations where the two electrons have the same parity. Thus, the required Hilbert space contains functions of the following form

$$\chi(\mathbf{r}_1, \mathbf{r}_2) = F_i(r_1)F_k(r_2)(j^\pi j^\pi 00), \tag{2}$$

where j is a positive number of the form $j = n + 1/2$, n is an integer and $\pi = \pm 1$.

The angular parts of any two different functions of (2) are orthogonal. Hence, off-diagonal matrix elements of any pure radial operator vanish. Since the following discussion is focused on finding off-diagonal matrix elements of the Hamiltonian, radial coordinates and radial operators are not always shown explicitly in expressions.

At this point one can use a given Hamiltonian and construct its matrix. Before doing this assignment one has to find a practical procedure that can be used for over-

coming the infinite number of configurations that can be obtained from the different values of n, j and π. For this purpose one organizes the configurations of (2) in an ascending order of j and examines a Hilbert subspace made of the first N_0 functions, where N_0 is a positive integer. Here a finite Hamiltonian matrix is obtained and one can diagonalize it, find the smallest eigenvalue E_0 and its associated eigenfunction Ψ_0. The quantities found here represent an approximation for the required solution. Let this approximate solution be denoted in this form

$$\{E_0, \Psi_0\}. \tag{3}$$

In order to evaluate the goodness of this approximation, one replaces N_0 by $N_1 = N_0+1$ and repeats the procedure. The new solution $\{E_1, \Psi_1\}$ is a better approximation because it relies on a larger Hilbert subspace. The difference between these solutions provides an estimate for the goodness of the solutions obtained. This procedure can be repeated for an increasing value of N_i. Thus, if a satisfactory approximation is reached for a certain value of N_i then one may terminate the calculation and use the solution obtained from this procedure as a good approximation to the accurate solution.

Now we are ready to examine the Hamiltonian's matrix elements. This examination demonstrates the advantage of using configurations as a basis for the Hilbert space. Thus, the angular part of the kinetic energy of each electron takes the form found for the hydrogen atom and only diagonal matrix elements do not vanish. The same result is obtained for the spherically symmetric radial potential operator Ze^2/r of the nucleus. It follows that off-diagonal matrix elements can be obtained only from the interaction between the two electrons. (This quantity does not exist for the one electron hydrogen atom and for this reason, each of the hydrogen atom eigenfunctions takes the form of a unique configuration.) In a full relativistic case the two-electron interaction takes the form of Breit interaction (see [10], p. 170), which contains the

instantaneous ordinary Coulomb term and a velocity-dependent term. The existence and the results of the Hamiltonian's off-diagonal matrix elements are the main objective of this discussion and it is shown below that for this purpose the examination of the relatively simple Coulomb term is enough.

Thus, one has to write the $1/r_{12}$ operator in a form that is suitable for a calculation that uses on the single particle independent variables $\mathbf{r}_1, \mathbf{r}_2$ of the configurations (2). This objective is achieved by carrying out a tensor expansion of the interaction (see [9], p. 208). For the specific case of the Coulomb interaction, the required expression is (see [11], p. 114)

$$\frac{1}{r_{12}} = \sum_{k=0}^{\infty} \frac{r_<^k}{r_>^{k+1}} P_k(\cos\theta_{12}). \tag{4}$$

Here $r_<$ and $r_>$ denote the smaller and the larger values of r_1 and r_2, respectively and θ_{12} is the angle between them. $P_k(\cos\theta_{12})$ is the Legendre polynomial of order k. At this point one uses the addition theorem for spherical harmonics (see [9], p. 113)

$$P_k(\cos\theta_{12}) = \frac{4\pi}{2k+1} \sum_{m=-k}^{k} (-1)^m Y_{k,-m}(\theta_1,\phi_1) Y_{k,m}(\theta_2,\phi_2) \tag{5}$$

and obtains an expansion of the Legendre polynomial $P_k(\cos\theta_{12})$ of (4) in terms of spherical harmonics that depend on single particle angular variables. This analysis shows how matrix elements can be obtained for a Hilbert space whose basis is made of functions that are an appropriate set of configurations.

At this point the wave functions of the Hilbert space basis as well as the Hamiltonian operator depend on the radial and the angular coordinates of single particle functions. The main objective of this section is to explain why the electronic states are described as a linear combination of configurations. It is shown above that the configurations of the Hilbert space basis are eigenfunctions of the operators representing the kinetic energy and the interaction with the spherically symmetric potential of the nucleus. Hence, the discussion is limited to the two particle operator (4) that depends on the expansion (5).

Let us find, for example, the off-diagonal matrix element of the configurations $((1\frac{1}{2}^{+})^2 00)$ and $((2\frac{3}{2}^{-})^2 00)$ of the Hilbert space basis (2). (As explained above, the radial coordinates do not contribute to the interaction between different configurations.) The discussion examines the 2-electron Coulomb interaction obtained for the upper (large) component of the Dirac spinor. Thus, $\frac{1}{2}^{+}$ is a spatial s-wave and $\frac{3}{2}^{-}$ is a spatial p-wave. The Wigner-Racah algebra provides explicit formulas for expressions that depend on the angular coordinates. Now, as stated above, the main objective of the discussion is to show that off-diagonal matrix elements do not vanish. For this purpose, only the main points of the calculation are written and readers can use explicit reference for working out the details.

The formal form of the angular component of the off-diagonal matrix element is

$$H_{ij} =< j_1 j_2 JM|\frac{1}{r_{12}}|j_1' j_2' JM > . \tag{6}$$

Here j_1, j_2 of the ket are angular momentum values of the first and the second electron, respectively and they are coupled to a total J, M. The bra has the same structure. In the particular case discussed here $J = M = 0$ and (6) takes the form

$$H_{ij} =< \tfrac{1}{2}\tfrac{1}{2}00|\frac{1}{r_{12}}|\tfrac{3}{2}\tfrac{3}{2}00 > . \tag{7}$$

The following points describe the steps used in the calculation of (7).

1. The Wigner-Eckart theorem shows that (6) can be cast into a product of a *Wigner 3j symbol* and a *reduced matrix element* (see [5], p. 117).

2. In (4), the expansion (5) of $1/r_{12}$ is a *scalar product of two tensors* (see [9], p. 128).

3. The reduced matrix element of such a scalar product can be put in the form of a product of a *Racah coefficient* and two reduced matrix elements that depend on the first and the second electron, respectively (see [5], p. 129).

4. Each of these reduces matrix elements takes the form $< slj||Y_k||sl'j' >$ where sl denote single particle spin and spatial angular momentum that are coupled to the particle's total angular momentum j. In the specific case discussed here it is $< \frac{1}{2}0\frac{1}{2}||Y_1||\frac{1}{2}1\frac{3}{2} >$. The value of the last expression can be readily obtained as a product of a square root of an integer and a Wigner $3j$ symbol (see [9], p. 521). The final value is

$$< \tfrac{1}{2}0\tfrac{1}{2}||Y_1||\tfrac{1}{2}1\tfrac{3}{2} >= \frac{-2}{\sqrt{4\pi}}. \tag{8}$$

This discussion shows that the Hamiltonian's off diagonal matrix elements do not vanish for the $J = 0$ ground state of the He atom. It means that a single configuration does not describe accurately this state. The next step is to carry out an explicit calculation and find out how good is the usage of a single configuration. This task has already been carried out [4] and it was proved that the description of the ground state of the He atom requires many configurations. Here radial and angular excitations take place and no single configuration plays a dominant role.

4. Discussion

Several aspects of the conclusion obtained in the previous section are discussed below.

Intuitively, the multiconfiguration structure of the ground state may be regarded as a mistake. Indeed, the ground state takes the lowest energy possible. Hence, how can a mixture of a lower energy state and a higher energy state yield a combined state whose energy is lower than either of the two single mono-configuration states? The answer to this question relies on a solid mathematical basis. Thus, a diagonalization of a Hermitian matrix reduces the lowest eigenvalue and increases the highest eigen-

value (see e.g. [12], pp. 420-423). Hence, *for a Hermitian matrix, any off-diagonal matrix element increases the difference between the corresponding diagonal elements.* It means that the smaller diagonal element decreases and the larger diagonal element increases. Since the Hamiltonian is a Hermitian operator, one concludes that if the Hilbert space basis yields a non-diagonal Hamiltonian matrix then the lowest eigenvalue "favors" eigenfunctions that are a linear combination of the Hilbert space basis functions.

It is shown in the previous section that the non-vanishing off-diagonal matrix elements stem from the two body Coulomb interaction between electrons. Thus, the tensor expansion of the interaction (4) casts the 2-body Coulomb interaction into a series of Legendre polynomials where $cos\theta_{12}$ is the polynomial's argument. Evidently, any physically meaningful interaction depends on the distance between the interacting particles. Hence, an expansion in terms of the Legendre polynomials can be obtained. This expansion proves that the mathematical procedure described in the previous section has a comprehensive validity (see [9], p. 208). Thus, what is found in the previous section for electrons in the He atom ground state also holds for quarks in the proton. Moreover, the proton is an extremely relativistic system of quarks and, as such, its spin-dependent interactions are expected to be quite strong. Evidently, spin dependent interactions make a contribution to off-diagonal matrix elements. On the basis of this conclusion, one infers that the proton's quark state must be described by a linear combination of many configurations.

A polarized proton experiment has been carried out where the instantaneous spin direction of quarks was measured [6]. The measurements have shown that *the total quark spin constitutes a rather small fraction of the proton's spin.* This result is in a complete agreement with the mathematical analysis carried out above. Thus, the relativistic proton dynamics indicates that the jj-coupling provides a better approach (and this is the reason for the usage of this notation here). In each quark configuration,

spin and spatial angular momentum are coupled to a total single particle j-value and the Clebsch-Gordan coefficients determine the portion of spin-up and spin-down of the quark. Next, The relativistic quark state indicates that, unlike the case of the hydrogen atom, the lower part of the Dirac spinor of quarks is quite large. As is well known, if in the upper part of a Dirac spinor is $l = j \pm 1/2$ then its lower part is $l = j \mp 1/2$. Hence, different Clebsch-Gordan coefficients are used for the upper and the lower parts of the Dirac spinor. Furthermore, in different configurations, different Clebsch-Gordan coefficients are used for the single particle coupling of the three quarks to the total proton's spin and the overall weight of the spin-up and spin-down components takes a similar value. This argument indicates that the outcome of [6] is quite obvious and that if the experiment would have yielded a different conclusion where *quarks carry the entire proton's spin then this result should have been regarded as a real crisis of fundamental quantum mechanical principles.* This discussion also shows that the quite frequently used description of the results of [6] as "the proton spin crisis" is unjustified.

Computers are based on quantum mechanical processes that take place in solid state devices. Hence, it is clear that people who have established the laws of quantum mechanics had no access to the computational power of computers. For this reason, several approximations have been contrived in order to get an insight into atomic structure. A method that deals with configurations is called *central field approximation* (see [13], p. 225). Here, for every electron, the actual field of all other electrons is replaced by an approximate spherically symmetric radial field. Evidently, as explained in the third section, such a radial field does not cause a configuration mixture and, in this approximation, a single configuration is used for describing atomic states. This approach is frequently used in a description of the Mendeleev's periodic table (see [13], pp. 240-247).

However, even in the early days of quantum mechanics, the central field approx-

imation has been regarded as an approximation and people have constructed mathematical tools for treating the multi-configuration atomic structure which is known as the Wigner-Racah algebra of angular momentum. These mathematical tools have been used in the early days of electronic computers [4] and the result is quite clear: *many configurations are required even for the simplest case of the ground state $J = 0$ of the 2-electron He atom and no single configuration plays a dominant role.* Today, this outcome is still known (see [11], p. 116) but unfortunately not widely known. Thus, [11] is based on lectures delivered in a chemistry department. On the other hand, the birth and the long duration of the idea concerning *the proton spin crisis* prove that this fundamental physical issue is indeed not widely known. This paper has been written for the purpose of improving the present status.

References:

* Email: elicomay@post.tau.ac.il

Internet site: http://www.tau.ac.il/∼elicomay

[1] E. A. Poe, *The Raven* (1845).

[2] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra*, (University Press, Cambridge, 1964).

[3] G. R. Taylor and R.G. Parr, Proc. Natl. Acad. Sci. USA **38**, 154 (1952).

[4] A. W. Weiss, Phys. Rev. **122**, 1826 (1961).

[5] Textbooks use the central field approximation and do not analyze the goodness of this argument. [11] (see p. 116) is a notable exception.

[6] J Ashman et al. (EMC) Phys. Lett. **B206**, 364 (1988).

[7] E. P. Wigner, Annals of Math., **40**, 149 (1939).

[8] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory*, (Harper & Row, New York, 1964). Pp. 44-53.

[9] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963).

[10] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two-Electron Atoms* (Springer, Berlin 1957).

[11] R. N. Zare, *Angular Momentum* (Wiley, New York, 1988).

[12] C. Cohen-Tannoudji, B. Diu and F. Laloe, *Quantum Mechanics* Vol. 1 (Wiley, New York,2005).

[13] L. D. Landau and E. M. Lifshitz *Quantum Mechanics* (Pergamon, London, 1959).